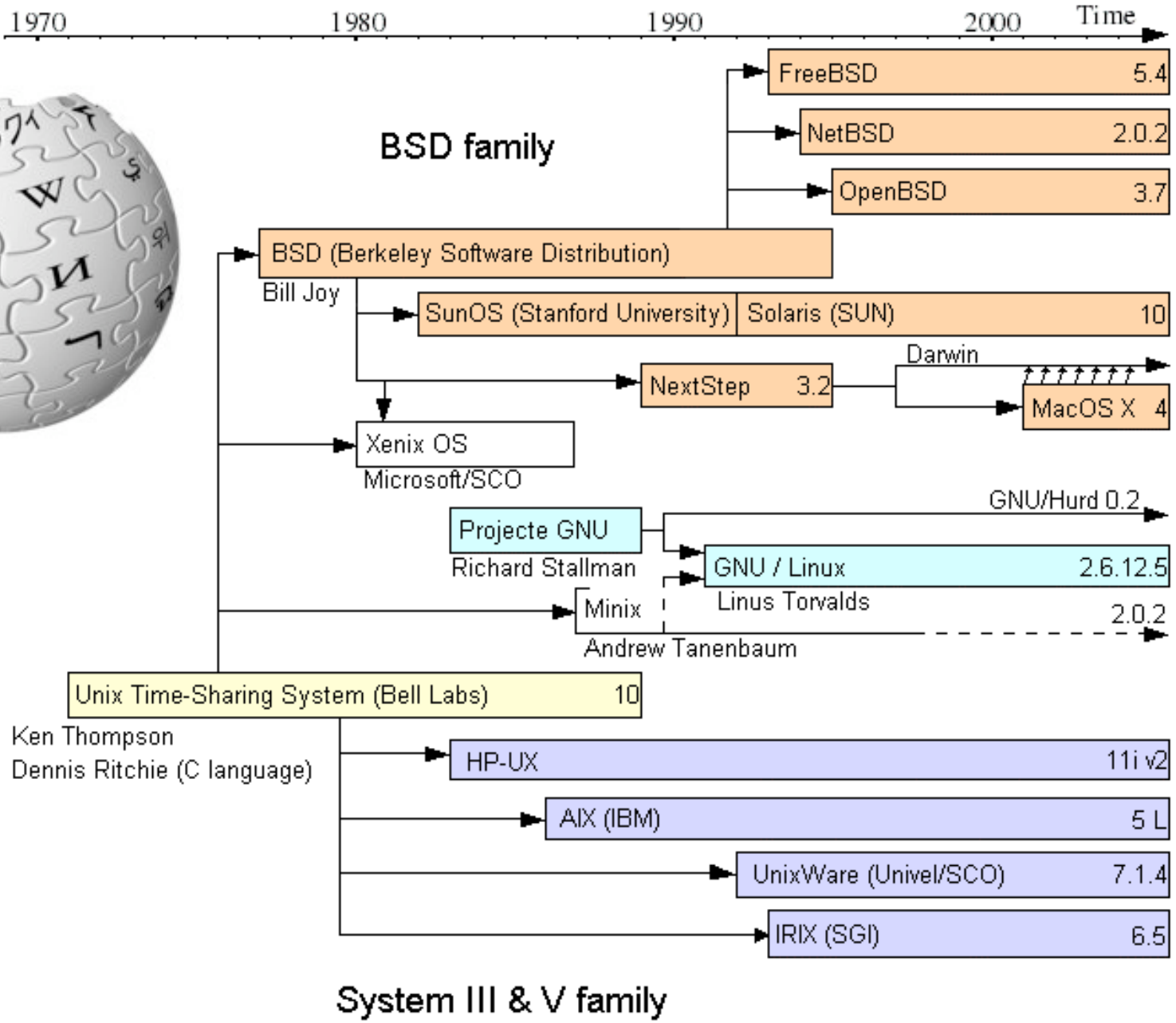
Unix


1970
1980
1990
2000
Time
BSD family
FreeBSD 5.4
NetBSD 2.0.2
OpenBSD 3.7
BSD (Berkeley Software Distribution)
Bill Joy
SunOS (Stanford University)
Solaris (SUN) 10
Darwin
NextStep 3.2
MacOS X 4
Xenix OS
Microsoft/SCO
GNU/Hurd 0.2
Projecte GNU
Richard Stallman
GNU / Linux 2.6.12.5
Linus Torvalds
Minix
2.0.2
Andrew Tanenbaum
Unix Time-Sharing System (Bell Labs) 10
Ken Thompson
Dennis Ritchie (C language)
HP-UX 11i v2
AIX (IBM) 5 L
UnixWare (Univel/SCO) 7.1.4
IRIX (SGI) 6.5
System III & V family

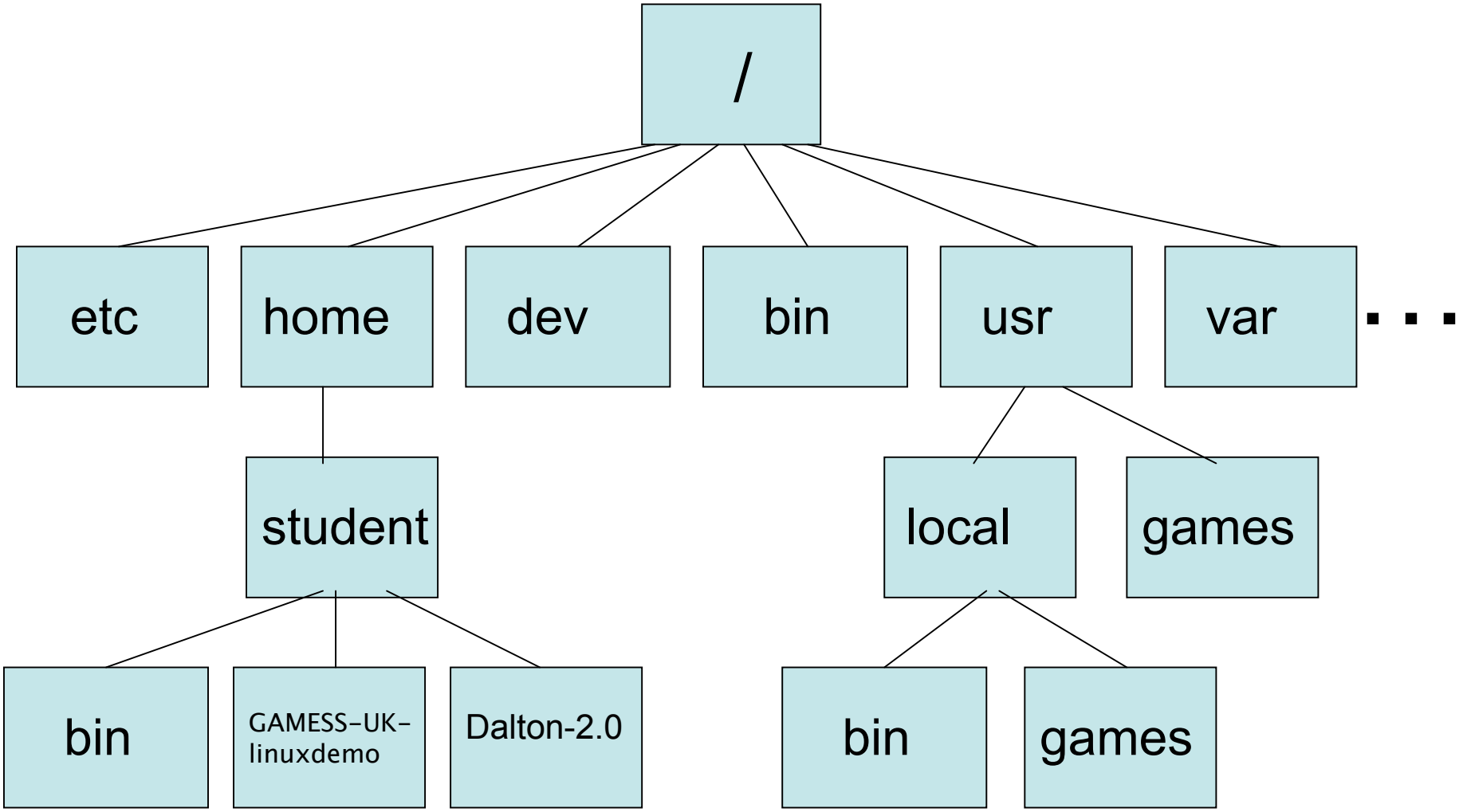
LINUX

1983- GNU* Project, towards a complete Unix-like operating system composed entirely of free software. 1990s, GNU had most of the necessary components - libraries, compilers, text editors, a Unix-like shell—except for the core component, the kernel. The GNU kernel proved difficult. *GNU = GNU's Not Unix

Linus Torvalds

1991, a kernel was begun as a hobby by Finnish university student Linus Torvalds (Helsinki). Torvalds originally used Minix, a simplified Unix-like system written by Andrew Tanenbaum (Amsterdam) for teaching. Tanenbaum did not permit others to extend his operating system, leading Torvalds to create a replacement for Minix.

Filesystem



Directories

Commands (no capitals)

- **man** (-k) command : Manual -k gives list of applicable pages
- **mkdir** path : Make directory
- **ls** (-al) path : List contents of directory
- **cd** path : go to directory
  ~ = your home; ../ = 1 up
- **pwd** : print working directory
- **cp** (-i) file1 file2 : copy file1 to file2
- **mv** (-i) file1 file2 : move file1 to file2
- **rm** (-i) file : remove (delete) a file or directory (-r)
- **cat** file : display a file
- **more** file : display file in pages (/,? Search; q quit
- **ps** : proces status
- **grep** pattern file : display lines containing the pattern
- ***name*** : run a procedure or a program
  e.g. gamess,vi,molden,nedit,install.csh

Programs-1

vi

Unix text editor / full screen - character commands

a : append; i : insert; o : open new line

- finish with ESC -

u : undo ; x : delete character; r : replace character;

R : replace part of line (finish ESC); [#]dd : delete line(s);

[#]yy : put line(s) in buffer; p : insert buffer; dw : delete word;

h : left; j : down; k : up; l : right; or arrow keys

ctrl-F : page-down; ctrl-B : page up

:q : quit; :x : save + quit; :n : line n; :set number : line-number

:[#,#]w file : write line range for file; :r file : read file in

/pattern : search for pattern; ?pattern : same backwards

Programs-2

In LINUX

have a look around in your system

On CD/Stick

GAMESS-UK : http://www.cfs.dl.ac.uk/docs/index.shtml

DALTON : http://www.kjemi.uio.no/software/dalton/dalton.html

MOLDEN : http://tc5.chem.uu.nl/MOLDEN_Manual/molden.html

Download yourself

Nedit :
http://download.fedora.redhat.com/pub/fedora/linux/core/3/i386/os/Fedora/RPMS/

Procedures/scripts

List of commands to be executed by a SHELL

```
#!/bin/csh
ls
```

The shell

The command

```
#!/bin/csh
cat << /END > out
echo 'Testing 1 2 3'
/END
ls
cat < out | more
chmod +x out
out
```

redirection

streaming

make *out* executable

run *out* (possibly ./out)

Resources on Web

tc5.chem.uu.nl

- **The GAMESS-UK 6.3 User Manual and Reference Guide**
- **The DALTON manual**
- **The MOLDEN manual**

-· **Terminal/werkstation Handleiding**
-· **QuantumChemie-dictaat Hoofdstuk 7**

- **Computing for Science (CFS)**
  - **Examples / Tutorials**

Gaussian Basis Set Library

QC

$$\text{LCAO} - \text{MO} \quad \psi = \sum_i c_i \phi_i$$

Moleculaire Orbital

Atomaire Orbital

$$H = \underbrace{\sum_i \left(-\tfrac{1}{2}\nabla_i^2 - \sum_A \frac{Z_A}{r_{iA}} \right)}_{1-electron} + \underbrace{\sum_{A<B} \frac{Z_A Z_B}{r_{AB}}}_{number} + \underbrace{\sum_{i<j} \frac{1}{r_{ij}}}_{2-electron}$$

$$F(i) = -\tfrac{1}{2}\nabla_i^2 - \sum_A \frac{Z_A}{r_{iA}} + \{\text{repulsie door andere elektronen}\}$$

Hartree-Fock

Voorbeeld Job

```
#!/bin/csh
gamess <<EOF
zmat angstrom
o
h 1 r
h 1 r 2 t
variables
r 1.04
t 104
end
EOF
```

chmod +x h2o

h2o >& h2o.out

Vragen :
- Is de Energie de som van de orbital energieen ?
- zie je een 1s orbital ?
- zie je een OH binding ?
- Hoeveel AO's zijn er ?

probeer toe te voegen
basis sto3g of basis dzp
runtype optimise of runtype infrared